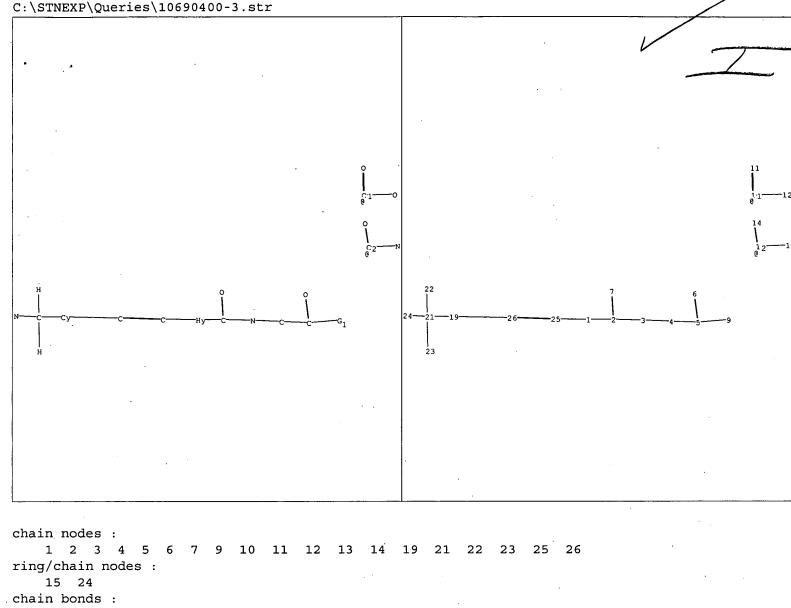
# **EAST Search History**

Ref #	Hits	Search Query	DBs	Default Operator	Plurals	Time Stamp
L7	28	pyridine-3-carboxamide near20 phenyl	US-PGPUB; USPAT	OR	OFF	2007/01/07 19:38
L8	66	pyridine-\$-carboxamide near20 phenyl	US-PGPUB; USPAT	OR	OFF	2007/01/07 19:33
L9	38	18 not 17	US-PGPUB; USPAT	OR	OFF	2007/01/07 19:35
L10	453	nicotinamide near20 phenyl	US-PGPUB; USPAT	OR	OFF	2007/01/07 19:39



1-2 1-25 2-3 2-7 3-4 4-5 5-6 5-9 10-11 10-12 13-14 13-15 19-21 19-26 21-22

21-23 21-24 25-26

exact/norm bonds :

1-2 1-25 2-3 2-7 3-4 5-6 5-9 10-11 10-12 13-14 13-15 19-21 19-26 21-24

exact bonds :

4-5 21-22 21-23 25-26

### G1:H,[\*1],[\*2]

Match level :

1:Atom 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 9:CLASS 10:CLASS 11:CLASS

12:CLASS 13:CLASS 14:CLASS 15:CLASS 19:Atom 21:CLASS 22:CLASS 23:CLASS 24:CLASS

25:CLASS 26:CLASS

Generic attributes :

1:

Saturation : Unsaturated Number of Carbon Atoms : less than 7 Type of Ring System : Monocyclic

19:

Saturation : Unsaturated Number of Carbon Atoms : less than 7

Type of Ring System : Monocyclic

Element Count :

. Node 1: Limited

N,N1

0,00

s,so

Node 19: Limited

N, NO-1

0,00

s,so

11/291216

\$%^STN;HighlightOn=;HighlightOff=;Version Version = STN Express 8.01a; => s 11

SAMPLE SEARCH INITIATED 23:54:24 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 107473 TO ITERATE

1.9% PROCESSED 2000 ITERATIONS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*INCOMPLETE\*\*

BATCH \*\*INCOMPLETE\*\*

PROJECTED ITERATIONS: 2130029 TO 2168891
PROJECTED ANSWERS: 1527 TO 2771

L2 2 SEA SSS SAM L1

Uploading C:\STNEXP\Queries\10690400-1.str



·2 ANSWERS



chain nodes :
1 2 3 4 5 6 7 9 10 11 12 20 21 22 23 24 25
ring/chain nodes :
26
chain bonds :
1-2 1-9 2-3 2-7 3-4 4-5 5-6 5-20 9-10 10-11 11-12 21-22 21-23 24-25
24-26
exact/norm bonds :
1-2 1-9 2-3 2-7 3-4 5-6 5-20 9-10 10-11 11-12 21-22 21-23 24-25 24-26
exact bonds :

G1:H,[\*1],[\*2]

Match level :

1:Atom 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 9:CLASS 10:CLASS 11:CLASS 12:Atom 20:CLASS 21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS

Generic attributes :

1:

4-5

Saturation : Unsaturated Number of Carbon Atoms : less than 7 Type of Ring System : Monocyclic

12:

Saturation : Unsaturated

Element Count :
Node 1: Limited

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S,S0
Node 12: Limited
   N, NO-2
   0,00
   S, S0
       STRUCTURE UPLOADED
L3
=> s 13
SAMPLE SEARCH INITIATED 23:58:55 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 107473 TO ITERATE
 1.9% PROCESSED
                   2000 ITERATIONS
                                                              0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01
FULL FILE PROJECTIONS:
                      ONLINE
                               **INCOMPLETE**
                       BATCH
                              **INCOMPLETE**
                          2130029 TO 2168891 .
PROJECTED ITERATIONS:
PROJECTED ANSWERS:
                                0 TO
                                           0
L4
             O SEA SSS SAM L3
=>
Uploading C:\STNEXP\Queries\10690400-2.str
                                                                       14
                                       31
chain nodes :
1 2 3 4 5 6 7 9 10 11 12 13 14 19 20 21
                                                      23 30
ring/chain nodes :
15 33
chain bonds :
1-2 1-19 2-3 2-7 3-4 4-5 5-6 5-9 10-11 10-12 13-14 13-15 19-23 20-21
20-23 21-30 30-31 30-32 30-33
exact/norm bonds :
1-2 1-19 2-3 2-7 3-4 5-6 5-9 10-11 10-12 13-14 13-15 19-23 20-21 20-23
 21-30 30-33
exact bonds :
4-5 30-31 30-32
```

11/291216

N, N1 O, O0

```
11/291216
G1:H,[*1],[*2]
Match level :
1:Atom 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 9:CLASS 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 19:CLASS 20:CLASS 21:Atom
23:CLASS 30:CLASS 31:CLASS 32:CLASS 33:CLASS
Generic attributes :
1:
Saturation
                      : Unsaturated
Number of Carbon Atoms : less than 7
Type of Ring System : Monocyclic
21:
Saturation
                     : Unsaturated
Number of Carbon Atoms : less than 7
Type of Ring System : Monocyclic
Element Count :
Node 1: Limited
   N,N1
   0,00
   S,SO
Node 21: Limited
   N, NO-1
   0,00
   S,SO
L5
       STRUCTURE UPLOADED
SAMPLE SEARCH INITIATED 00:06:58 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -
                                  97389 TO ITERATE
                                                                0 ANSWERS
  2.1% PROCESSED
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INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01
FULL FILE PROJECTIONS:
                               **INCOMPLETE**
                       ONLINE
                       BATCH
                              **INCOMPLETE**
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1929261 TO 1966299

0

O TO

PROJECTED ITERATIONS:

O SEA SSS SAM L5

Uploading C:\STNEXP\Queries\10690400-3.str

PROJECTED ANSWERS:

L6

chain nodes : 1 2 3 4 5 6 7 9 10 11 12 19 21 22 23 25 26 13 14 ring/chain nodes : 15 24 chain bonds : 1-2 1-25 2-3 2-7 3-4 4-5 5-6 5-9 10-11 10-12 13-14 13-15 19-21 19-26 21-22 21-23 21-24 25-26 exact/norm bonds : 1-2 1-25 2-3 2-7 3-4 5-6 5-9 10-11 10-12 13-14 13-15 19-21 19-26 21-24 exact bonds : 4-5 21-22 21-23 25-26

G1:H,[\*1],[\*2]

Match level:
1:Atom 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 9:CLASS 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 19:Atom 21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 6:CLASS 19:Atom 21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 26

Saturation : Unsaturated
Number of Carbon Atoms : less than 7
Type of Ring System : Monocyclic
19:

Saturation : Unsaturated
Number of Carbon Atoms : less than 7
Type of Ring System : Monocyclic

Element Count : Node 1: Limited N,N1 O,O0 S,S0

Node 19: Limited N,N0-1 O,O0

S,S0

11/291216

L7 STRUCTURE UPLOADED

=> s 17

SAMPLE SEARCH INITIATED 00:09:49 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED -6522 TO ITERATE

30.7% PROCESSED 2000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED) SEARCH TIME: 00.00.01

O ANSWERS

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

\*\*COMPLETE\*\* BATCH

PROJECTED ITERATIONS: 125598 TO 135282 PROJECTED ANSWERS: 0 TO

0 SEA SSS SAM L7 L8

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FULL SEARCH INITIATED 00:09:58 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED -132491 TO ITERATE

100.0% PROCESSED 132491 ITERATIONS 17 ANSWERS

SEARCH TIME: 00.00.06

17 SEA SSS FUL L7

=> file caplus

COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION 178.59 178.38

FULL ESTIMATED COST

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FILE COVERS 1907 - 26 Dec 2006 VOL 146 ISS 1 FILE LAST UPDATED: 24 Dec 2006 (20061224/ED)

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http://www.cas.org/infopolicy.html

=> s 19

L10 2 L9

=> d l10 1-2 bib abs hitstr

L10 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN

2003:340386 CAPLUS AN

139:100906

### 11/291216

- TI Benzoylalanine-Derived Ketoamides Carrying Vinylbenzyl Amino Residues: Discovery of Potent Water-Soluble Calpain Inhibitors with Oral Bioavailability
- AU Lubisch, Wilfried; Beckenbach, Edith; Bopp, Sabina; Hofmann, Hans-Peter; Kartal, Arzu; Kaestel, Claudia; Lindner, Tanja; Metz-Garrecht, Marion; Reeb, Jutta; Regner, Ferdinand; Vierling, Michael; Moeller, Achim
- CS Neuroscience Discovery Research, Abbott GmbH & Co. KG, Ludwigshafen, D-67008, Germany
- SO Journal of Medicinal Chemistry (2003), 46(12), 2404-2412 CODEN: JMCMAR; ISSN: 0022-2623
- PB American Chemical Society
- DT Journal
- LA English
- OS CASREACT 139:100906
- Novel benzoylalanine-derived ketoamides were prepared and evaluated for AΒ calpain I inhibition. Derivs. carrying vinylbenzyl amino residues in the P2-P3 region inhibited calpain in nanomolar concns. and thus represent a novel class of nonpeptidic calpain inhibitors. Selected examples exhibited an improved pharmacokinetic profile including improved water-solubility and metabolic stability. In particular, these calpain inhibitors showed oral bioavailability in rats as demonstrated by N-(1-benzyl-2-carbamoyl-2-oxoethyl)-2-(E-2-(4-benzyl-2-carbamoyl-2-oxoethyl)diethylaminomethylphenyl)ethen-1-yl]benzamide. The closely related derivative N-(1-carbamoyl-1-oxohex-1-yl)-2-[E-2-(4-dimethylaminomethylphenyl)-ethen-1-yl)yl]benzamide (I) was evaluated for neuroprotective efficacy after exptl. traumatic brain injury in a fluid percussion model in rats. When administered after injury, I reduced the number of damaged neurons by 41%, and this result would be in line with the suggested neuroprotective efficacy of calpain inhibition.
- IT 247218-50-4P
  - RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation of N-(2-vinylbenzoyl)- and N-(2-vinyl-3-pyridinecarbonyl)-alaninamides as calpain inhibitors) .

- RN 247218-50-4 CAPLUS
- CN 3-Pyridinecarboxamide, N-[3-amino-2,3-dioxo-1-(phenylmethyl)propyl]-2[(1E)-2-[4-[(diethylamino)methyl]phenyl]ethenyl]-, dihydrochloride (9CI)
  (CA INDEX NAME)

Double bond geometry as shown.

●2 HCl

RE.CNT 51 THERE ARE 51 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1999:691085 CAPLUS

DN 131:310835

```
Preparation of cysteine protease inhibitors for therapeutic use
TΙ
     Lubisch, Wilfried; Moller, Achim; Treiber, Hans-Jorg; Knopp, Monika
ΙN
     BASF Aktiengesellschaft, Germany
SO
     PCT Int. Appl., 52 pp.
     CODEN: PIXXD2
DT
     Patent
LA
     German
FAN.CNT 1
     PATENT NO.
                          KIND
                                 DATE
                                              APPLICATION NO.
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                                 _____
                                              -----
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                          A2
                                 19991028
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                                                                      19990420
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     WO 9954310
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             KZ, LT, LV, MK, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TR, UA, US,
         ZA, AM, AZ, KG, MD, TJ, TM
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                           т .
                                 20040415
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PRAI DE 1998-19818615
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                                 19980420
     WO 1999-EP2633
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     US 2000-673089
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                                 20001011
OS
     MARPAT 131:310835
GΙ
```

$$(R^2)n$$
  $R^3$   
 $A-B-D-Y-CO-NH-CH-CO-R^4$   $I$ 

$$\begin{array}{c} \text{H}_2\text{C} \longrightarrow \text{Ph} \\ \text{H}_2\text{C} \longrightarrow \text{Ph} \\ \text{Me}_2\text{N} \longrightarrow \text{CH}_2 - \text{p-C}_6\text{H}_4 - \text{C} \longrightarrow \text{C-o-C}_6\text{H}_4 - \text{CO} \longrightarrow \text{NH} \end{array}$$

AB The invention relates to cysteine protease inhibitors of the general formula [(I); A = -(CH2)p-R1; R1 = pyrrolidine, morpholine, piperidine, -NR5R6, (N-substituted)piperazine; R5, R6 = independently H, alkyl, cyclohexyl, cyclopentyl, (CH2)nPh, where Ph may be R6-substituted; p = 1-2; B = (substituted) Ph, pyridyl, pyrimidyl or pyridazyl; D = bond, -(CH2)m-, -CH:CH-, -C.tplbond.C-; R2 = Cl, Br, F, alkyl, NHCO alkyl, NHSO2 alkyl, NO2, -O-alkyl or NH2; R3 = alkyl which can carry a (substituted) Ph

ring, indolyl ring or cyclohexyl ring; Y = Ph, pyridine, pyrimidine or pyrazine; R4 = H, COOR9 or CO-Z, where Z = NR10R11; R9,R10,R11 = (independently) H, (unsubstituted) (unbranched) alkyl; n = 0-2 and m = 0-4]. Thus, Et 2-bromo-benzoate and dimethyl(4-vinylbenzyl)amine were reacted, de-esterified, and the free acid intermediate reacted with (S)-phenylalaninol to give an intermediate which was reduced to give aldehyde (II) in 88% yield. Title compds. showed good results as inhibitors of calpain I and II or cathepsin B in a variety of in vivo and in vitro tests (no data given).

In vitro tests (no data given).

247218-29-7P 247218-39-9P 247218-43-5P 247218-44-6P 247218-45-7P 247218-46-8P 247218-47-9P 247218-48-0P 247218-49-1P 247218-50-4P 247218-51-5P 247218-69-5P 247219-00-7P 247219-02-9P 247219-05-2P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of as cysteine protease inhibitors for therapeutic use)

RN 247218-29-7 CAPLUS

CN 3-Pyridinecarboxamide, 2-[(1E)-2-[4-[(dimethylamino)methyl]phenyl]ethenyl]-N-[(1S)-1-formyl-2-phenylethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

RN 247218-39-9 CAPLUS

CN 3-Pyridinecarboxamide, N-[3-amino-2,3-dioxo-1-(phenylmethyl)propyl]-2[(1E)-2-[4-[(dimethylamino)methyl]phenyl]ethenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 247218-43-5 CAPLUS

CN 3-Pyridinecarboxamide, N-[3-amino-2,3-dioxo-1-(phenylmethyl)propyl]-2-[(1E)-2-[4-[(diethylamino)methyl]phenyl]ethenyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ &$$

RN 247218-44-6 CAPLUS

CN 3-Pyridinecarboxamide, N-[1-(aminooxoacetyl)pentyl]-2-[(1E)-2-[4-[(diethylamino)methyl]phenyl]ethenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

$$\begin{array}{c|c} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & &$$

RN 247218-45-7 CAPLUS

CN 3-Pyridinecarboxamide, N-[1-(aminooxoacetyl)pentyl]-2-[(1E)-2-[4-[(4-methyl-1-piperazinyl)methyl]phenyl]ethenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 247218-46-8 CAPLUS

CN 3-Pyridinecarboxamide, N-[3-amino-2,3-dioxo-1-(phenylmethyl)propyl]-2[(1E)-2-[4-(1-pyrrolidinylmethyl)phenyl]ethenyl]- (9CI) (CA INDEX NAME)

RN 247218-47-9 CAPLUS

CN 3-Pyridinecarboxamide, N-[1-(aminooxoacetyl)pentyl]-2-[(1E)-2-[4-(1-piperidinylmethyl)phenyl]ethenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 247218-48-0 CAPLUS

CN 3-Pyridinecarboxamide, N-[3-amino-2,3-dioxo-1-(phenylmethyl)propyl]-2- [(1E)-2-[4-(1-piperidinylmethyl)phenyl]ethenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 247218-49-1 CAPLUS

CN 3-Pyridinecarboxamide, N-[3-amino-2,3-dioxo-1-(phenylmethyl)propyl]-2- [(1E)-2-[4-(4-morpholinylmethyl)phenyl]=thenyl]- (9CI) (CA INDEX NAME)

RN 247218-50-4 CAPLUS

CN 3-Pyridinecarboxamide, N-[3-amino-2,3-dioxo-1-(phenylmethyl)propyl]-2[(1E)-2-[4-[(diethylamino)methyl]phenyl]ethenyl]-, dihydrochloride (9CI)
(CA INDEX NAME)

Double bond geometry as shown.

### ●2 HC1

RN 247218-51-5 CAPLUS

CN 3-Pyridinecarboxamide, N-[3-amino-2,3-dioxo-1-(phenylmethyl)propyl]-2-[(1E)-2-[4-[(dimethylamino)methyl]phenyl]ethenyl]-, dihydrochloride (9CI) (CA INDEX NAME)

Double bond geometry as shown.

$$H_2N$$
 $O$ 
 $Ph$ 
 $N$ 
 $N$ 
 $N$ 
 $N$ 
 $N$ 
 $N$ 
 $N$ 

### ●2 HCl

RN 247218-69-5 CAPLUS

CN 3-Pyridinecarboxamide, N-(3-amino-1-methyl-2,3-dioxopropyl)-2-[(1E)-2-[4-(4-morpholinylmethyl)phenyl]ethenyl]-, dihydrochloride (9CI) (CA INDEX NAME)

Double bond geometry as shown.

### ●2 HCl

RN 247219-00-7 CAPLUS

CN 3-Pyridinecarboxamide, N-[1-(aminooxoacetyl)pentyl]-2-[(1E)-2-[4-[(4-methyl-1-piperazinyl)methyl]phenyl]ethenyl]-, dihydrochloride (9CI) (CA INDEX NAME)

Double bond geometry as shown.

### ●2 HCl

RN 247219-02-9 CAPLUS

CN 3-Pyridinecarboxamide, N-[3-amino-2,3-dioxo-1-(phenylmethyl)propyl]-2-[(1E)-2-[4-[(4-methyl-1-piperazinyl)methyl]phenyl]ethenyl]-, dihydrochloride (9CI) (CA INDEX NAME)

### ● 2 HCl

RN 247219-05-2 CAPLUS

CN 3-Pyridinecarboxamide, N-[3-amino-2,3-dioxo-1-(phenylmethyl)propyl]-2[(1E)-2-[4-(4-morpholinylmethyl)phenyl]ethenyl]-, dihydrochloride (9CI)
(CA INDEX NAME)

Double bond geometry as shown.

### ●2 HCl

=> log hCOST IN U.S. DOLLARS SINCE FILE TOTAL **ENTRY** SESSION FULL ESTIMATED COST 10.68 189.27 DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL ENTRY SESSION CA SUBSCRIBER PRICE -1.50-1.50

SESSION WILL BE HELD FOR 120 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 00:10:48 ON 26 DEC 2006

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ring nodes :
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ring/chain nodes :
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chain bonds :
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   19-22
ring bonds :
   24-25 24-29 25-26 26-27 27-28 28-29
exact/norm bonds :
   1-6 1-2 2-3 4-5 4-7 8-9 8-10 11-12 11-13 17-19 19-22
exact bonds :
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normalized bonds :
   24-25 24-29 25-26 26-27 27-28 28-29
isolated ring systems :
   containing 24 :
```

G1:H,[\*1],[\*2]

```
Match level:
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 12:CLASS 13:CLASS 17:Atom 19:CLASS 20:CLASS 21:CLASS 22:CLASS 23:CLASS
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24:Atom 25:CLASS 26:Atom 27:Atom 28:Atom 29:Atom

Generic attributes :

17:

Saturation : Unsaturated Number of Carbon Atoms : less than 7

Element Count :

Node 17: Limited

N, NO-1

0,00

S,S0

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FULL SEARCH INITIATED 23:48:56 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 11521 TO ITERATE

100.0% PROCESSED 11521 ITERATIONS

50 ANSWERS

172.76

SEARCH TIME: 00.00.01

L5 50 SEA SSS FUL L3

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION

172.10

FULL ESTIMATED COST

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FILE COVERS 1907 - 7 Jan 2007 VOL 146 ISS 3 FILE LAST UPDATED: 5 Jan 2007 (20070105/ED)

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http://www.cas.org/infopolicy.html

=> s 15

L6 3 L5

=> d 16 1-3 bib abs hitstr

- L6 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN
- AN 2003:340386 CAPLUS
- DN 139:100906
- TI Benzoylalanine-Derived Ketoamides Carrying Vinylbenzyl Amino Residues: Discovery of Potent Water-Soluble Calpain Inhibitors with Oral Bioavailability
- AU Lubisch, Wilfried; Beckenbach, Edith; Bopp, Sabina; Hofmann, Hans-Peter; Kartal, Arzu; Kaestel, Claudia; Lindner, Tanja; Metz-Garrecht, Marion; Reeb, Jutta; Regner, Ferdinand; Vierling, Michael; Moeller, Achim
- CS Neuroscience Discovery Research, Abbott GmbH & Co. KG, Ludwigshafen, D-67008, Germany
- SO Journal of Medicinal Chemistry (2003), 46(12), 2404-2412 CODEN: JMCMAR; ISSN: 0022-2623
- PB American Chemical Society
- DT Journal
- LA English
- OS CASREACT 139:100906
- AB Novel benzoylalanine-derived ketoamides were prepared and evaluated for calpain I inhibition. Derivs. carrying vinylbenzyl amino residues in the

P2-P3 region inhibited calpain in nanomolar concns. and thus represent a novel class of nonpeptidic calpain inhibitors. Selected examples exhibited an improved pharmacokinetic profile including improved water-solubility and metabolic stability. In particular, these calpain inhibitors showed oral bioavailability in rats as demonstrated by N-(1-benzyl-2-carbamoyl-2-oxoethyl)-2-[E-2-(4diethylaminomethylphenyl)ethen-1-yl]benzamide. The closely related derivative N-(1-carbamoyl-1-oxohex-1-yl)-2-[E-2-(4-dimethylaminomethylphenyl)-ethen-1yl]benzamide (I) was evaluated for neuroprotective efficacy after exptl. traumatic brain injury in a fluid percussion model in rats. When administered after injury, I reduced the number of damaged neurons by 41%, and this result would be in line with the suggested neuroprotective efficacy of calpain inhibition.

IT 247218-50-4P

> RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation of N-(2-vinylbenzoyl)- and N-(2-vinyl-3-pyridinecarbonyl)alaninamides as calpain inhibitors)

247218-50-4 CAPLUS RN

3-Pyridinecarboxamide, N-[3-amino-2,3-dioxo-1-(phenylmethyl)propyl]-2-CN [(1E)-2-[4-[(diethylamino)methyl]phenyl]ethenyl]-, dihydrochloride (9CI) (CA INDEX NAME)

Double bond geometry as shown.

#### HCl **9**2

#### THERE ARE 51 CITED REFERENCES AVAILABLE FOR THIS RECORD RE.CNT 51 ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 2 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN. L6

AN 1999:691085 CAPLUS

DN 131:310835

ΤI Preparation of cysteine protease inhibitors for therapeutic use

ΙN Lubisch, Wilfried; Moller, Achim; Treiber, Hans-Jorg; Knopp, Monika

PA BASF Aktiengesellschaft, Germany

SO PCT Int. Appl., 52 pp.

CODEN: PIXXD2

DT Patent

LA German

FAN.CNT 1 PATENT NO. KIN							KIND DATE				A DDT	ICAT:	DATE						
	FAILNI NO.					RIND DATE													
	PI WO 9954310			A2		19991028			WO 1999-EP2633						19990420				
		WO .9954310			A3		20000217												
			W:	AL,	ΑU,	BG,	BR,	BY,	CA,	CN,	CZ,	GE,	HR,	HU,	ID,	ΙL,	IN,	JP,	KR,
				ΚZ,	LT,	LV,	MK,	MX,	NO,	NZ,	PL,	RO,	RU,	SG,	SI,	SK,	TR,	UA,	US,
				ZA,	AM,	ΑZ,	KG,	MD,	ТJ,	TM									
			RW:	AT,	BE,	CH,	CY,	DE,	DK,	ES,	FI,	FR,	GB,	GR,	ΙE,	ΙT,	LU,	MC,	NL,

			PT,	SE															
	CA	CA 2328396					19991028			CA 1999-2328396						19990420 .			
	ΑU	AU 9939276					19991108			AU 1999-39276						19990420			
	BR	R 9909774				Α	20001219			BR 1999-9774						19990420			
	EΡ	10736	A2	20010207			EP 1999-922108						19990420						
	ĒΡ	P 1073641					20040414												
		R:	AT,	BE,	CH,	DE,	DK,	ES,	FR,	GB, G	SR.	, IT,	LI,	LU,	NL,	SE,	PT,	ΙE,	
			SI,	FI,	RO														
	TR 200003068					Т2	20010321 TR 2000-200003068							19990420					
	ни 200102732					A2		2001	1228	HU	ни 2001-2732						19990420		
	JΡ	JP 2002512231				T		2002	0423	JE	JP 2000-544649						19990420		
	ΑT	AT 264310				${f T}$		2004	0415	. AT	AT 1999-922108					19990420			
	ES	ES 2220061				Т3		2004	1201	ES	ES 1999-922108					19990420			
	US	US 6753327				В1		2004	0622	US 2000-673089						20001011			
	BG	10487	73			Α		2001	0731	BG	BG 2000-104873					20001017			
	ЮN	20000	0526	63		Α		2000	1019	NC	NO 2000-5263					20001019			
	HR	20000	0078	37		A1		2001	0831	HF	₹ :	2000-	787			2	0001	117	
	ZA	20000	0673	19		Α		2002	0815	ZF	ZA 2000-6719						20001117		
	US	20040	8256	69		A1		2004	0429	US	US 2003-690400						20031020		
PRAI	DE 1998-19818615			ĵ	Α		1998	0420											
	WO	1999-	-EP26	633		W		1999	0420										
	US	2000-	-6730	089		A3		2000	1011										
OS MARPAT 131:310835																			
GI																			

$$\begin{array}{c} \text{H}_2\text{C} - \text{Ph} \\ \text{H}_2\text{C} - \text{Ph} \\ \text{H}_2\text{C} - \text{Ph} \\ \text{H}_2\text{C} - \text{Ph} \\ \text{CHO} \end{array}$$

The invention relates to cysteine protease inhibitors of the general AB. formula [(I); A = -(CH2)p-R1; R1 = pyrrolidine, morpholine, piperidine, -NR5R6, (N-substituted)piperazine; R5, R6 = independently H, alkyl, cyclohexyl, cyclopentyl, (CH2)nPh, where Ph may be R6-substituted; p = 1-2; B = (substituted) Ph, pyridyl, pyrimidyl or pyridazyl; D = bond, -(CH2)m-, -CH:CH-, -C.tplbond.C-; R2 = Cl, Br, F, alkyl, NHCO alkyl, NHSO2 alkyl, NO2, -O-alkyl or NH2; R3 = alkyl which can carry a (substituted) Ph ring, indolyl ring or cyclohexyl ring; Y = Ph, pyridine, pyrimidine or pyrazine; R4 = H, COOR9 or CO-Z, where Z = NR10R11; R9,R10,R11 = (independently) H, (unsubstituted) (unbranched) alkyl; n = 0-2 and m = 0-10-4]. Thus, Et 2-bromo-benzoate and dimethyl(4-vinylbenzyl)amine were reacted, de-esterified, and the free acid intermediate reacted with (S)-phenylalaninol to give an intermediate which was reduced to give aldehyde (II) in 88% yield. Title compds. showed good results as inhibitors of calpain I and II or cathepsin B in a variety of in vivo and in vitro tests (no data given).

IT 247218-29-7P 247218-39-9P 247218-43-5P
 247218-44-6P 247218-45-7P 247218-46-8P
 247218-47-9P 247218-48-0P 247218-49-1P
 247218-50-4P 247218-51-5P 247218-69-5P
 247219-00-7P 247219-02-9P 247219-05-2P
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);

BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of as cysteine protease inhibitors for therapeutic use)

RN 247218-29-7 CAPLUS

CN 3-Pyridinecarboxamide, 2-[(1E)-2-[4-[(dimethylamino)methyl]phenyl]ethenyl]-N-[(1S)-1-formyl-2-phenylethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

RN 247218-39-9 CAPLUS

CN 3-Pyridinecarboxamide, N-[3-amino-2,3-dioxo-1-(phenylmethyl)propyl]-2[(1E)-2-[4-[(dimethylamino)methyl]phenyl]ethenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

$$H_2N$$
 $O$ 
 $Ph$ 
 $N$ 
 $N$ 
 $E$ 
 $N$ 
 $N$ 
 $N$ 

RN 247218-43-5 CAPLUS

CN 3-Pyridinecarboxamide, N-[3-amino-2,3-dioxo-1-(phenylmethyl)propyl]-2[(1E)-2-[4-[(diethylamino)methyl]phenyl]ethenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 247218-44-6 CAPLUS

CN 3-Pyridinecarboxamide, N-[1-(aminooxoacetyl)pentyl]-2-[(1E)-2-[4-[(diethylamino)methyl]phenyl]ethenyl]- (9CI) (CA INDEX NAME)

$$H_2N$$
 $O$ 
 $NEt_2$ 

RN 247218-45-7 CAPLUS

CN 3-Pyridinecarboxamide, N-[1-(aminooxoacetyl)pentyl]-2-[(1E)-2-[4-[(4-methyl-1-piperazinyl)methyl]phenyl]ethenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

Me N NH O NH
$$_2$$

RN 247218-46-8 CAPLUS

Double bond geometry as shown.

RN 247218-47-9 CAPLUS

CN 3-Pyridinecarboxamide, N-[1-(aminooxoacetyl)pentyl]-2-[(1E)-2-[4-(1-piperidinylmethyl)phenyl]ethenyl]- (9CI) (CA INDEX NAME)

RN 247218-48-0 CAPLUS

CN 3-Pyridinecarboxamide, N-[3-amino-2,3-dioxo-1-(phenylmethyl)propyl]-2- [(1E)-2-[4-(1-piperidinylmethyl)phenyl]ethenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 247218-49-1 CAPLUS

CN 3-Pyridinecarboxamide, N-[3-amino-2,3-dioxo-1-(phenylmethyl)propyl]-2[(1E)-2-[4-(4-morpholinylmethyl)phenyl]ethenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 247218-50-4 CAPLUS

CN 3-Pyridinecarboxamide, N-[3-amino-2,3-dioxo-1-(phenylmethyl)propyl]-2[(1E)-2-[4-[(diethylamino)methyl]phenyl]ethenyl]-, dihydrochloride (9CI)
(CA INDEX NAME)

### ●2 HCl

RN 247218-51-5 CAPLUS

CN 3-Pyridinecarboxamide, N-[3-amino-2,3-dioxo-1-(phenylmethyl)propyl]-2[(1E)-2-[4-[(dimethylamino)methyl]phenyl]ethenyl]-, dihydrochloride (9CI)
(CA INDEX NAME)

Double bond geometry as shown.

$$H_2N$$
 $O$ 
 $Ph$ 
 $N$ 
 $N$ 
 $N$ 
 $N$ 

### ●2 HC1

RN 247218-69-5 CAPLUS

CN 3-Pyridinecarboxamide, N-(3-amino-1-methyl-2,3-dioxopropyl)-2-[(1E)-2-[4-(4-morpholinylmethyl)phenyl]ethenyl]-, dihydrochloride (9CI) (CA INDEX NAME)

RN 247219-00-7 CAPLUS

CN 3-Pyridinecarboxamide, N-[1-(aminooxoacetyl)pentyl]-2-[(1E)-2-[4-[(4-methyl-1-piperazinyl)methyl]phenyl]ethenyl]-, dihydrochloride (9CI) (CA INDEX NAME)

Double bond geometry as shown.

### ● 2 HCl

RN 247219-02-9 CAPLUS

CN 3-Pyridinecarboxamide, N-[3-amino-2,3-dioxo-1-(phenylmethyl)propyl]-2[(1E)-2-[4-[(4-methyl-1-piperazinyl)methyl]phenyl]ethenyl]-,
dihydrochloride (9CI) (CA INDEX NAME)

Double bond geometry as shown.

### ●2 HC1

RN 247219-05-2 CAPLUS

CN 3-Pyridinecarboxamide, N-[3-amino-2,3-dioxo-1-(phenylmethyl)propyl]-2[(1E)-2-[4-(4-morpholinylmethyl)phenyl]ethenyl]-, dihydrochloride (9CI)
(CA INDEX NAME)

PRAI DE 1998-19817462

WO 1999-EP2632

MARPAT 131:299460

### ●2 HCl

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ANSWER 3 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN
L6
     1999:691081 CAPLUS
ΑN
DN
     131:299460
     Preparation of piperazinylnicotinamides and related compounds as calpain
ΤI
     and cathepsin inhibitors.
     Lubisch, Wilfried; Moller, Achim; Treiber, Hans-Jorg; Knopp, Monika
ΙN
     BASF Aktiengesellschaft, Germany
PA
SO
     PCT Int. Appl., 103 pp.
     CODEN: PIXXD2
DT
     Patent
LA
     German
FAN.CNT 1
                                             APPLICATION NO.
     PATENT NO.
                          KIND
                                 DATE
     ______
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     WO 9954305
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                                 19991028
                                             WO 1999-EP2632
                                                                      19990420
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             KZ, LT, LV, MK, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TR, UA, US,
             ZA, AM, AZ, KG, MD, TJ, TM
         RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL,
             PT, SE
     CA 2328440
                                 19991028
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                           Α1
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                                                                      19990420
     AU 9938190
     BR 9909773
                           Α
                                 20001219
                                             BR 1999-9773
                                                                      19990420
     TR 200003004
                           T2
                                              TR 2000-200003004
                                                                      19990420
                                 20010221
                                             EP 1999-920710
                                                                      19990420
     EP 1082308
                          Α1
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                          DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE,
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             SI, FI, RO
     HU 200101599
                           A2
                                 20010928
                                             HU 2001-1599
                                                                      19990420
     JP 2002512229
                           Т
                                 20020423
                                              JP 2000-544646
                                                                      19990420
     US 6562827
                           В1
                                 20030513
                                             US 2000-647681
                                                                      20001003
                                                                      20001018
                                             NO 2000-5237
     NO 2000005237
                           Α
                                 20001018
                                             HR 2000-764
     HR 2000000764
                           A1
                                 20010630
                                                                      20001110
                                             BG 2000-104961
                                                                      20001117
     BG 104961
                           Α
                                 20010531
     ZA 2000006712
                           Α
                                 20020923
                                              ZA 2000-6712
                                                                      20001117
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AB A(CH2)xR1R2BCONHCHR3COR4 [A = (substituted) piperazinyl, homopiperazinyl, hexahydroazepinyl, piperidinyl, pyrrolidinyl; B = Ph, pyridyl, pyrimidinyl, pyrazinyl, pyridazinyl; R1, R2 = H, alkyl, alkoxy, OH, Cl, F, Br, iodo, CF3, NO2, NH2, cyano, CO2H, alkoxycarbonyl, alkylcarbonylamino, etc.; R3 = alkyl, methylthioalkyl, cyclohexylalkyl, cyclopentylalkyl, cycloheptylalkyl, phenylalkyl, pyridylalkyl, pyrimidinylalkyl, pyridazinylalkyl, indolylalkyl, etc.; R4 = H, COR8; R8 = OR9, NR9R10; R9 = H, alkyl; R10 = H, (substituted) alkyl], were prepared for treatment of

19980420 19990420

Α

W

neurodegenerative disease (no data). Thus, Me chloronicotinate, 4-pyridylpiperazine, and 18-crown-6 were heated at 100° in DMF to give 82% Me 2-[4-(pyrid-4-yl)piperazin-1-yl]nicotinate. The latter was saponified with LiOH in THF/H2O and the acid was stirred with Et3N and Na2SO4 in CH2Cl2/DMF; phenylalanino, HOBT, and EDC were added at 0° followed by stirring overnight at room temperature to give 2-[4-(pyrid-4-yl)piperazin-1-yl]nicotinic acid-N-(3-phenylpropan-1-ol-2-yl)amide. This was stirred with SO3.pyridine and Et3N in Me2SO to give 2-[4-(pyrid-4-yl)piperazin-1-yl]nicotinic acid-N-(3-phenylpropan-1-al-2-yl)amide.

IT 247116-90-1P 247116-91-2P 247116-92-3P 247116-93-4P 247116-94-5P 247116-95-6P 247116-96-7P 247116-98-9P 247117-01-7P 247117-02-8P 247117-04-0P 247117-05-1P 247117-10-8P 247117-12-0P 247117-13-1P 247117-14-2P 247117-15-3P 247117-17-5P 247117-19-7P 247117-20-0P 247117-21-1P 247117-22-2P 247117-24-4P 247117-28-8P 247117-35-7P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of piperazinylnicotinamides and related compds. as calpain and cathepsin inhibitors)

RN 247116-90-1 CAPLUS

CN 3-Pyridinecarboxamide, N-(1-formyl-2-phenylethyl)-2-[4-(phenylmethyl)-1-piperazinyl]- (9CI) (CA INDEX NAME)

RN 247116-91-2 CAPLUS

CN 3-Pyridinecarboxamide, N-(1-formyl-2-phenylethyl)-2-[4-(2-pyridinylmethyl)-1-piperazinyl]- (9CI) (CA INDEX NAME)

RN 247116-92-3 CAPLUS

CN 3-Pyridinecarboxamide, N-(1-formyl-2-phenylethyl)-2-[4-(3-pyridinylmethyl)-1-piperazinyl]- (9CI) (CA INDEX NAME)

RN 247116-93-4 CAPLUS

CN 3-Pyridinecarboxamide, N-(1-formyl-2-phenylethyl)-2-[4-(4-pyridinylmethyl)-1-piperazinyl]- (9CI) (CA INDEX NAME)

RN 247116-94-5 CAPLUS

CN 3-Pyridinecarboxamide, N-(1-formyl-2-phenylethyl)-2-[hexahydro-4-(phenylmethyl)-1H-1,4-diazepin-1-yl]- (9CI) (CA INDEX NAME)

RN 247116-95-6 CAPLUS

CN 3-Pyridinecarboxamide, N-(1-formyl-2-phenylethyl)-2-[hexahydro-4-(2-pyridinylmethyl)-1H-1,4-diazepin-1-yl]- (9CI) (CA INDEX NAME)

RN 247116-96-7 CAPLUS

CN 3-Pyridinecarboxamide, N-(1-formyl-2-phenylethyl)-2-[hexahydro-4-(4-pyridinylmethyl)-1H-1,4-diazepin-1-yl]- (9CI) (CA INDEX NAME)

RN 247116-98-9 CAPLUS

CN 3-Pyridinecarboxamide, N-(1-formyl-2-phenylethyl)-2-[4-[(2-methoxyphenyl)methyl]-1-piperazinyl]- (9CI) (CA INDEX NAME)

RN 247117-01-7 CAPLUS

CN 3-Pyridinecarboxamide, 2-[4-[[4-(dimethylamino)phenyl]methyl]hexahydro-1H-1,4-diazepin-1-yl]-N-(1-formyl-2-phenylethyl)- (9CI) (CA INDEX NAME)

RN 247117-02-8 CAPLUS

CN 3-Pyridinecarboxamide, 2-[4-[(2-fluorophenyl)methyl]-1-piperazinyl]-N-(1-formyl-2-phenylethyl)- (9CI) (CA INDEX NAME)

RN 247117-04-0 CAPLUS

CN 3-Pyridinecarboxamide, N-[3-amino-2,3-dioxo-1-(phenylmethyl)propyl]-2-[hexahydro-4-(2-pyridinylmethyl)-1H-1,4-diazepin-1-yl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \text{CH}_2\text{-Ph} \\ \parallel & \parallel & \parallel \\ \text{C-NH-CH-C-C-NH}_2 \\ \hline \downarrow N & & \text{N-} \\ \parallel & \parallel & \parallel \\ & & \text{O} & \text{O} \\ \end{array}$$

RN 247117-05-1 CAPLUS

CN 3-Pyridinecarboxamide, N-(1-formyl-2-phenylethyl)-2-[4-[(4-methoxyphenyl)methyl]-1-piperazinyl]- (9CI) (CA INDEX NAME)

RN 247117-06-2 CAPLUS

CN 3-Pyridinecarboxamide, N-(1-formyl-2-phenylethyl)-2-[hexahydro-4-[(4-methoxyphenyl)methyl]-1H-1,4-diazepin-1-yl]- (9CI) (CA INDEX NAME)

RN 247117-07-3 CAPLUS

CN 3-Pyridinecarboxamide, 2-[4-[(4-butoxyphenyl)methyl]-1-piperazinyl]-N-(1-formyl-2-phenylethyl)- (9CI) (CA INDEX NAME)

CN 3-Pyridinecarboxamide, N-(1-formyl-2-phenylethyl)-2-[4-[(2-methylphenyl)methyl]-1-piperazinyl]- (9CI) (CA INDEX NAME)

RN 247117-11-9 CAPLUS

CN 3-Pyridinecarboxamide, N-(1-formyl-2-phenylethyl)-2-[4-[(3-methylphenyl)methyl]-1-piperazinyl]- (9CI) (CA INDEX NAME)

RN 247117-12-0 CAPLUS

CN 3-Pyridinecarboxamide, N-(1-formyl-2-phenylethyl)-2-[4-[(4-methylphenyl)methyl]-1-piperazinyl]- (9CI) (CA INDEX NAME)

RN 247117-13-1 CAPLUS

CN Benzoic acid, 4-[[4-[3-[[(1-formyl-2-phenylethyl)amino]carbonyl]-2-pyridinyl]-1-piperazinyl]methyl]-, methyl ester (9CI) (CA INDEX NAME)

RN 247117-14-2 CAPLUS

CN 3-Pyridinecarboxamide, N-(1-formyl-2-phenylethyl)-2-[hexahydro-4-(3-pyridinylmethyl)-1H-1,4-diazepin-1-yl]- (9CI) (CA INDEX NAME)

RN 247117-15-3 CAPLUS

CN 3-Pyridinecarboxamide, N-[3-amino-2,3-dioxo-1-(phenylmethyl)propyl]-2-[4-(phenylmethyl)-1-piperazinyl]-, dihydrochloride (9CI) (CA INDEX NAME)

### ●2 HCl

RN 247117-17-5 CAPLUS

CN 3-Pyridinecarboxamide, N-[1-(aminooxoacetyl)pentyl]-2-[4-(phenylmethyl)-1-piperazinyl]- (9CI) (CA INDEX NAME)

RN 247117-19-7 CAPLUS

CN 3-Pyridinecarboxamide, N-[2,3-dioxo-1-(phenylmethyl)-3-[[2-(1-piperidinyl)ethyl]amino]propyl]-2-[4-(phenylmethyl)-1-piperazinyl]- (9CI) (CA INDEX NAME)

RN 247117-20-0 CAPLUS

CN 3-Pyridinecarboxamide, N-[2,3-dioxo-1-(phenylmethyl)-3-[[2-(2-pyridinyl)ethyl]amino]propyl]-2-[4-(phenylmethyl)-1-piperazinyl]- (9CI) (CA INDEX NAME)

RN 247117-21-1 CAPLUS

CN 3-Pyridinecarboxamide, N-[3-[[3-(4-methyl-1-piperazinyl)propyl]amino]-2,3-dioxo-1-(phenylmethyl)propyl]-2-[4-(phenylmethyl)-1-piperazinyl]- (9CI) (CA INDEX NAME)

RN 247117-22-2 CAPLUS

CN 3-Pyridinecarboxamide, N-[3-[[3-(diethylamino)propyl]amino]-2,3-dioxo-1-(phenylmethyl)propyl]-2-[4-(phenylmethyl)-1-piperazinyl]- (9CI) (CA INDEX NAME)

RN 247117-24-4 CAPLUS

CN 3-Pyridinecarboxamide, 2-[4-[3-[(dimethylamino)methyl]-2-pyridinyl]-1-piperazinyl]-N-(1-formyl-2-phenylethyl)-, (2E)-2-butenedioate (1:3) (9CI) (CA INDEX NAME)

CM 1

CRN 247117-23-3 CMF C27 H32 N6 O2

CM 2

CRN 110-17-8 CMF C4 H4 O4

Double bond geometry as shown.

RN 247117-28-8 CAPLUS

CN 3-Pyridinecarboxamide, 2-[4-[[4-(dimethylamino)phenyl]methyl]-1-piperazinyl]-N-(1-formyl-2-phenylethyl)- (9CI) (CA INDEX NAME)

CN 3-Pyridinecarboxamide, N-[3-amino-2,3-dioxo-1-(phenylmethyl)propyl]-4-[4-(phenylmethyl)-1-piperazinyl]- (9CI) (CA INDEX NAME)

RN 247117-33-5 CAPLUS

CN 3-Pyridinecarboxamide, N-(1-formylbutyl)-2-[4-(phenylmethyl)-1-piperazinyl]- (9CI) (CA INDEX NAME)

RN 247117-34-6 CAPLUS

CN 3-Pyridinecarboxamide, N-[1-formyl-2-(1H-indol-3-yl)ethyl]-2-[4-(phenylmethyl)-1-piperazinyl]- (9CI) (CA INDEX NAME)

RN 247117-35-7 CAPLUS

CN 3-Pyridinecarboxamide, N-[1-formyl-2-(1H-indol-3-yl)ethyl]-2-[hexahydro-4-(2-pyridinylmethyl)-1H-1,4-diazepin-1-yl]- (9CI) (CA INDEX NAME)

## RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> file caold		
COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	16.28	189.04
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-2.34	-2.34

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FILE COVERS 1907-1966 FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

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COST IN U.S. DOLLARS
SINCE FILE TOTAL
ENTRY SESSION
O.45 189.49

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)
SINCE FILE TOTAL
ENTRY SESSION

CA SUBSCRIBER PRICE

0.00

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SESSION WILL BE HELD FOR 120 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 23:49:44 ON 07 JAN 2007